Enumeration of Equicolourable Trees

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Abstract: A tree, being a connected acyclic graph, can be bicoloured in two ways, which differ from each other by exchange of the colours. We shall say that a tree is *equicolourable* if these bicolourings assign the two colours to equal numbers of vertices. Labelled equicoloured trees have been enumerated several times in the literature, and from this result it is easy to enumerate labelled equicolourable trees. The result is that the probability that a randomly chosen n-vertex labelled tree is equicolourable is asymptotically just twice the probability that its vertices would be equicoloured if they were assigned colours by independent unbiased coin flips. Our goal in this paper is the enumeration of unlabelled equicolourable trees (that is, trees up to isomorphism), both exactly (in terms of generating functions) and asymptotically. We treat both the rooted and unrooted versions of this problem, and conclude that in either case the probability that a randomly chosen n-vertex unlabelled tree is equicolourable is asymptotically 1.40499... times as large as the probability that it would be equicoloured if its vertices were assigned colours by independent unbiased coin flips.

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1. Introduction

Our goal in this paper is the enumeration, exact and asymptotic, of certain kinds of trees. A tree can have its vertices bicoloured (so that adjacent vertices are oppositely coloured) in exactly two ways, which differ by exchange of the colours. We shall be particularly interested in those trees for which equal numbers of vertices are assigned the two colours; we call such trees *equicolourable*. (It is tempting to call them "balanced," but the term "balanced trees" is already in use for several kinds of objects different from those treated here.)

Our solution to this problem also yields the enumeration of *equicoloured* trees; that is, equicolourable trees that have been assigned one of their two equitable bicolourings. For trees that are labelled or rooted, the distinction between enumerating "equicolourable" and "equicoloured" trees is trivial, for there are exactly two equicoloured trees for each equicolourable one. But when we enumerate unlabelled and unrooted trees, the distinction is significant, for to enumerate equicoloured trees we must count each equicolourable tree once or twice according as there is or is not a colour-exchanging automorphism of the tree.

Our approach to these problems can be sketched as follows. For the sake of example we consider unlabelled but rooted trees. We consider bicolourings of these trees (not necessarily equicolourings) in which the vertices are coloured red and blue, and in which the root is coloured red. Specifying the colour of the root fixes the colours of all other vertices. Let $r_{l,m}$ denote the number of such red-rooted trees with l red and m blue vertices. Let

$$r(x,y) = \sum_{l\ge 1, m\ge 0} r_{l,m}\ x^l y^m$$

be the generating function for red-rooted trees, in which the coefficent of $x^l y^m$ is the number of trees with l red vertices and m blue vertices. Then $r(y,x)$ is the generating function for blue-rooted trees.

By standard combinatorial methods, we obtain a functional equation determining $r(x,y)$. Then we make the substitutions $x = z\exp(i\vartheta)$ and $y = z\exp(-i\vartheta)$, and thus define

$$\begin{aligned} r_\vartheta(z) &= r\big(z\exp(i\vartheta), z\exp(-i\vartheta)\big) \\ &= \sum_{\substack{n\ge 1 \\ k\equiv n \pmod 2}} r_{(n+k)/2,(n-k)/2}\ z^n \exp(ik\vartheta), \end{aligned}$$

which is a trigonometric series in which the coefficient of $z^n \exp(ik\vartheta)$ is the number of red-rooted trees with n vertices and k more red vertices than blue vertices. In fact, it will be technically more convenient to work with the related series

$$\begin{aligned} c_\vartheta(z) &= \frac{r_\vartheta(z) + r_{-\vartheta}(z)}{2}, \\ &= \sum_{\substack{n \geq 1 \\ k \equiv n \pmod 2}} r_{(n+k)/2,(n-k)/2}\, z^n \cos(k\vartheta), \end{aligned}$$

in which red-rooted and blue-rooted trees are each counted with weight one-half. In deriving the functional equation for this series, the conjugate series

$$\begin{aligned} s_\vartheta(z) &= \frac{r_\vartheta(z) - r_{-\vartheta}(z)}{2i}, \\ &= \sum_{\substack{n \geq 1 \\ k \equiv n \pmod 2}} r_{(n+k)/2,(n-k)/2}\, z^n \sin(k\vartheta) \end{aligned}$$

will play an auxiliary role. Next we use the formula

$$\frac{1}{2\pi} \int_0^{2\pi} \cos(k\vartheta)\, d\vartheta = \begin{cases} 1, & \text{if } k = 0, \\ 0, & \text{if } k \neq 0, \end{cases}$$

to segregate the terms corresponding to equicoloured trees from the others. Specifically, the generating function

$$r^*(z) = \frac{1}{2\pi} \int_0^{2\pi} c_\vartheta(z)\, d\vartheta$$

enumerates equicolourable rooted trees, since we have counted both the red- and blue-rooted versions of the tree, each with weight one-half. This method of extracting the diagonal terms from a bivariate power series appears to be new in the combinatorial literature. Hautus and Klarner [H] give a method based on contour integration. Our method is of course equivalent, but more convenient in the case at hand because of the role of the conjugate trigonometric series indicated above.

Finally, by standard analytic methods, we determine the asymptotic behaviour of the coefficients in $r^*(z)$. To do this we determine, for each ϑ in the interval $[0, 2\pi)$ of integration, the behaviour of the coefficients in $c_\vartheta(z)$; then we estimate the integral of the resulting expression. Since $c_\vartheta(z)$ is periodic in ϑ with period 2π, the integral can be taken over any interval of length 2π. In fact, since the greatest contributions to the integral come when ϑ is near one of two points, 0 and π, it will be technically convenient to take the interval of integration to be $[-\pi/2, 3\pi/2)$, which has 0 and π as interior points.

The enumeration of equicolourable labelled trees (either rooted or unrooted) follows easily from the enumeration of equicoloured labelled trees, which has been dealt with already in the literature. Nevertheless, in Section 2 we shall solve this problem again using methods that will extend later to the unlabelled case. This will provide a testing ground for our methods, in a setting where the outcome is known in advance. The result is that the probability that a randomly chosen n-vertex labelled tree is equicolourable is asymptotically just twice the probability that its vertices would be equicoloured if they were assigned colours by independent unbiased coin flips (which is $\binom{n}{n/2}/2^n \sim (2/\pi n)^{1/2}$ for n even, and 0 for n odd.) In Section 3, we shall enumerate equicolourable rooted unlabelled trees. Finally, in Section 4, we shall enumerate equicolourable unrooted unlabelled trees. For both rooted and unrooted trees, we conclude that the probability that a randomly chosen n-vertex unlabelled tree is equicolourable is asymptotically $1.40499\ldots$ times as large as the probability that it would be equicoloured if its vertices were assigned colours by independent unbiased coin flips.

2. Labelled Trees

It was Cayley [C5] who in 1889 first stated that the number of labelled trees on n vertices is n^{n-2}, though this result is implicit in earlier related work by Sylvester [S2] in 1857 and Borchardt [B] in 1860. Many proofs of this result are now known; see Moon [M1,M2]. The one most relevant here, due to Pólya [P1,P2], is as follows.

A labelled tree on n vertices can be rooted in exactly n different ways, so it will suffice to show that the number R_n of rooted labelled trees is n^{n-1}. Let

$$R(z) = \sum_{n\geq 1} \frac{R_n}{n!}$$

be the exponential generating function for rooted labelled trees. Pólya's *component principle* states that if $F(z)$ is the exponential generating function for labelled "components," then

$$G(z) = \exp F(z) \tag{2.1}$$

is the exponential generating function for labelled structures comprising zero or more disjoint components. Since a rooted tree comprises a root (enumerated by z) together with zero or more disjoint rooted trees (the subtrees adjacent to the root, enumerated by $\exp R(z)$), $R(z)$ satisfies the functional equation

$$R(z) = z \exp R(z). \tag{2.2}$$

From this equation, Lagrange's inversion formula gives $n^{n-1}/n!$ as the coefficient $[z^n]R(z)$ of z^n in $R(z)$. Thus we conclude that $R_n = n^{n-1}$, as claimed.

Since we shall work later with functional equations to which Lagrange's inversion formula cannot be applied, it will be instructive to see how even without it the asymptotic behaviour of the coefficients of $R(z)$ can be extracted from (2.2).

The key idea will be the use of Darboux's lemma to deduce the asymptotic behaviour of the coefficients from the nature of the singularities of $R(z)$. To find the singularities of $R(z)$ as a function of z, we write (2.2) as $\Phi\big(z, R(z)\big) = 0$, where

$$\Phi(z, w) = z \exp w - w.$$

To locate the singularities, we calculate

$$\frac{\partial}{\partial w}\Phi(z, w) = \Phi(z, w) + w - 1.$$

The singularities occur when this derivative and $\Phi(z, w)$ vanish simultaneously for $w = R(z)$. This happens only for $w = W_0 = R(Z_0) = 1$ and $z = Z_0 = 1/e$. To expand $R(z)$ in the neighbourhood of $z = Z_0$, we calculate

$$\frac{\partial^2}{\partial w^2}\Phi(z, w) = \frac{\partial}{\partial w}\Phi(z, w) + 1 = \Phi(z, w) + w$$

and

$$\frac{\partial}{\partial z}\Phi(z, w) = \big(\Phi(z, w) + w\big)/z.$$

Then we have

$$\frac{\partial^2}{\partial w^2}\Phi(z, w)\Big|_{w=W_0, z=Z_0} = 1$$

and

$$\frac{\partial}{\partial z}\Phi(z, w)\Big|_{w=W_0, z=Z_0} = 1/Z_0,$$

so that

$$\begin{aligned}\Phi(z, w) = \frac{1}{2}(w - W_0)^2 + O\big((w - W_0)^3\big)\\ - (1 - z/Z_0) + O\big((w - W_0)(1 - z/Z_0)\big) + O\big((1 - z/Z_0)^2\big).\end{aligned}$$

Thus at $z = Z_0$, $R(z)$ has a branch point of order 2, and an expansion of the form

$$R(z) = A(z) + B(z)(1 - z/Z_0)^{1/2}$$

where $A(z) = 1 + O(z)$ and $B(z) = -2^{1/2} + O(z)$ are analytic functions of z. Applying Darboux's lemma [D] (see also Knuth and Wilf [K]), we conclude that $[z^n]R(z)$ is asymptotic to $e^n/n^{3/2}(2\pi)^{1/2}$, and thus by Stirling's formula that R_n is asymptotic to n^{n-1}.

The problem of enumerating equicoloured labelled trees will be reduced to the problem of enumerating certain "rooted spanning trees." Let $K_{l,m} = (V, W, E)$ denote the complete bipartite graph with l red vertices $V = \{v_1, \ldots, v_l\}$, m blue vertices $W = \{w_1, \ldots, w_m\}$, and lm edges E. (Each edge is an unordered pair comprising one vertex from V and one from W.) Let $R_{l,m}$ denote the number of red-rooted spanning trees in $K_{l,m}$, that is, the number of spanning trees in which one of the red vertices has been distinguished as the root. Since each unrooted spanning tree in $K_{l,m}$ can be assigned a red root in exactly l different ways, the number of unrooted spanning trees in $K_{l,m}$ is $R_{l,m}/l$. In particular, there are $R_{m,m}/m$ unrooted spanning trees in $K_{m,m}$. Each equicoloured labelled tree on $n = 2m$ vertices gives rise to $\binom{2m}{m}$ unrooted spanning trees in $K_{m,m}$, since the $2m$ vertices $U = \{u_1, \ldots, u_{2m}\}$ can be partitioned into m red vertices V and m blue vertices W in exactly $\binom{2m}{m}$ different ways. Thus there are $\binom{2m}{m}R_{m,m}/m$ equicoloured labelled trees. Since each equicolourable labelled tree can be equicoloured in exactly two different ways, there are $\binom{2m}{m}R_{m,m}/2m$ equicolourable labelled trees on $n = 2m$ vertices. (There are of course no equicolourable trees with an odd number of vertices.)

The problem of enumerating equicolourable labelled trees reduces to the problem of enumerating red-rooted spanning trees in $K_{l,m}$. This latter problem has been solved by Austin [A] (see also Scoins [S1] and Glicksman [G]), who showed that $R_{l,m} = l^m m^{l-1}$. The proofs of Austin and Scoins are based on the following idea.

Let

$$R(x, y) = \sum_{l \geq 1, m \geq 0} \frac{R_{l,m}}{l!\, m!}$$

be the bivariate exponential generating function for red-rooted spanning trees in $K_{l,m}$. The component principle analogous to (2.1) for bivariate exponential generating functions is

$$G(x, y) = \exp F(x, y),$$

where $F(x, y)$ is the generating function for components and $G(x, y)$ is the generating function for structures comprising zero or more disjoint components. Since a rooted spanning tree with a red root comprises a red root (enumerated by x) together with zero or more

disjoint rooted trees (which have blue roots, and are thus enumerated by $R(y,x)$), $R(x,y)$ satisfies the functional equation

$$R(x,y) = x \exp R(y,x). \tag{2.3}$$

Austin and Scoins use this equation, together with Lagrange's inversion formula, to show that the coefficient $[x^l y^m]R(x,y)$ of $x^l y^m$ in $R(x,y)$ is $l^m m^{l-1}/l!\,m!$. Thus $R_{l,m} = l^m m^{l-1}$, as claimed. In particular, $R_{m,m} = m^{2m-1}$. As before, we shall derive this asymptotic behaviour without using Lagrange's inversion formula.

As indicated in the introduction, we begin by making the substitutions $x = z\exp(i\vartheta)$ and $y = z\exp(-i\vartheta)$, and thus defining

$$R_\vartheta(z) = R\big(z\exp(i\vartheta), z\exp(-i\vartheta)\big). \tag{2.4}$$

From (2.3) and (2.4) we obtain

$$R_\vartheta(z) = z\exp\big(i\vartheta + R_{-\vartheta}(z)\big) \tag{2.5}$$

as the functional equation satisfied by $R_\vartheta(z)$.

We shall be interested in real values of ϑ, and it will turn out that the singularities of $R_\vartheta(z)$ occur at real values of z. It will be convenient therefore to work with relatives of $R_\vartheta(z)$ that are real when ϑ and z are real. Thus we define

$$C_\vartheta(z) = \frac{R_\vartheta(z) + R_{-\vartheta}(z)}{2} \tag{2.6}$$

and

$$S_\vartheta(z) = \frac{R_\vartheta(z) - R_{-\vartheta}(z)}{2i}. \tag{2.7}$$

We can find the functional equations satisfied by $C_\vartheta(z)$ and $S_\vartheta(z)$ by substituting (2.5) into (2.6) and (2.7), then substituting $R_\vartheta(z) = C_\vartheta(z) + iS_\vartheta(z)$ and $R_{-\vartheta(z)} = C_\vartheta(z) - iS_\vartheta(z)$ into the result, to obtain

$$C_\vartheta(z) = z\exp C_\vartheta(z)\,\cos\big(\vartheta - S_\vartheta(z)\big) \tag{2.8}$$

and

$$S_\vartheta(z) = z\exp C_\vartheta(z)\,\sin\big(\vartheta - S_\vartheta(z)\big). \tag{2.9}$$

We shall need to determine the singularities of $C_\vartheta(z)$ as a function of z with ϑ fixed. To find them, we square (2.8) and (2.9), and add them to obtain

$$C_\vartheta(z)^2 + S_\vartheta(z)^2 = z^2 \exp\bigl(2C_\vartheta(z)\bigr).$$

We then use this result to eliminate $S_\vartheta(z)$ from (2.8), obtaining

$$C_\vartheta(z) = z \exp C_\vartheta(z) \cos\Bigl(\vartheta - \bigl(z^2 \exp\bigl(2C_\vartheta(z)\bigr) - C_\vartheta(z)^2\bigr)^{1/2}\Bigr).$$

This equation can be written as $\Phi_\vartheta\bigl(z, C_\vartheta(z)\bigr) = 0$, where

$$\Phi_\vartheta(z,w) = z \exp w \cos\Bigl(\vartheta - \bigl(z^2 \exp(2w) - w^2\bigr)^{1/2}\Bigr) - w.$$

To locate the singularities of $C_\vartheta(z)$, we calculate

$$\frac{\partial}{\partial w}\Phi_\vartheta(z,w) = \Phi_\vartheta(z,w) - 1 + z^2 \exp(2w).$$

The singularites occur when this derivative and $\Phi(z,w)$ vanish simultaneously for $w = C_\vartheta(z)$, so that we have

$$Z_\vartheta^\pm = \pm \exp -C_\vartheta(Z_\vartheta^\pm). \tag{2.10}$$

Substituting this relation into (2.8) and (2.9) yields

$$C_\vartheta(Z_\vartheta^\pm) = \pm \cos\bigl(\vartheta - S_\vartheta(Z_\vartheta^\pm)\bigr), \tag{2.11}$$

and

$$S_\vartheta(Z_\vartheta^\pm) = \pm \sin\bigl(\vartheta - S_\vartheta(Z_\vartheta^\pm)\bigr), \tag{2.12}$$

where of course we must take the same sign throughout all three equations.

The solution to (2.11) and (2.12), and similar pairs of equations, can be expressed in terms of the coordinates of the cycloid curve, defined parametrically by

$$X(t) = t + \sin t$$
$$Y(t) = \cos t.$$

This curve is the locus of a marked point on a hoop of radius 1 that rolls without slipping on the line $Y = -1$. We define the cycloid function by

$$\operatorname{cyc}\vartheta = Y\bigl(X^{-1}(\vartheta)\bigr).$$

This function is periodic with period 2π. It has a crest $\operatorname{cyc}\vartheta = 1 - \vartheta^2/8 + O(\vartheta^4)$ in the neighbourhood of $\vartheta = 0$, and a cusp $\operatorname{cyc}\vartheta = -1 + (9/2)^{1/3}(\vartheta - \pi)^{2/3}$ in the neighbourhood of $\vartheta = \pi$. (Some discussions of the cycloid assume that the hoop rolls on the line $Y = 0$, or that $\vartheta = 0$ corresponds to a cusp rather than a crest, or both.) We shall also need the cocycloid curve, defined by

$$X(t) = t + \sin t$$
$$Z(t) = \sin t,$$

and the cocycloid function, defined by

$$\operatorname{cocyc}\vartheta = Z\big(X^{-1}(\vartheta)\big).$$

This function represents the lag of the centre of the hoop behind the marked point. It is also periodic with period 2π, and it has inflexions at $\vartheta = 0$ and $\vartheta = \pi$, with expansions $\operatorname{cocyc}\vartheta = \vartheta/2 + O(\vartheta^3)$ and $\operatorname{cocyc}\vartheta = -6^{1/3}(\vartheta - \pi)^{1/3} + O(\vartheta - \pi)$ in the neighbourhoods of these points, respectively. Finally, we have the identity $\operatorname{cyc}^2\vartheta + \operatorname{cocyc}^2\vartheta = 1$.

These definitions allow us to solve (2.11) and (2.12). We have $W_\vartheta^+ = C_\vartheta(Z_\vartheta^+) = \operatorname{cyc}\vartheta$, so that

$$Z_\vartheta^+ = \exp -\operatorname{cyc}\vartheta. \tag{2.13}$$

Taking the minus sign in (2.11) and (2.12) is equivalent to shifting ϑ by π, so we have

$$Z_\vartheta^- = -\exp -\operatorname{cyc}(\vartheta - \pi). \tag{2.14}$$

It may appear paradoxical that we have found two singularities for $C_\vartheta(z)$, whereas there was only one for $R(z) = C_0(z)$. The resolution of this paradox will appear shortly.

To expand $C_\vartheta(z)$ in the neighbourhood of $z = Z_\vartheta^+$, we calculate

$$\frac{\partial^2}{\partial w^2}\Phi_\vartheta(z,w) = \frac{\partial}{\partial w}\Phi_\vartheta(z,w) + 2z^2\exp(2w) = \Phi_\vartheta(z,w) - 1 + 3z^2\exp(2w)$$

and

$$\frac{\partial}{\partial z}\Phi_\vartheta(z,w) = \big(\Phi_\vartheta(z,w) + w + z^2\exp(2w)\big)/z.$$

We then have

$$\frac{\partial^2}{\partial w^2}\Phi_\vartheta(z,w)\big|_{w=W_\vartheta^+, z=Z_\vartheta^+} = 2$$

and

$$\frac{\partial}{\partial z}\Phi_\vartheta(z,w)\big|_{w=W_\vartheta^+, z=Z_\vartheta^+} = (1 + W_\vartheta^+)/Z_\vartheta^+,$$

so that

$$\Phi_\vartheta(z,w) = (w - W_\vartheta^+)^2 + O\big((w - W_\vartheta^+)^3\big) \\ - (1 + W_\vartheta^+)(1 - z/Z_\vartheta^+) + O\big((w - W_\vartheta^+)(1 - z/Z_\vartheta^+)\big) + O\big((1 - z/Z_\vartheta^+)^2\big).$$

Thus at Z_ϑ^+, $C_\vartheta(z)$ has a branch point of order 2, and an expansion of the form

$$C_\vartheta(z) = A_\vartheta^+(z) + B_\vartheta^+(z)(1 - z/Z_\vartheta^+)^{1/2},$$

where $A_\vartheta^+(z) = \operatorname{cyc}\vartheta + O(z - Z_\vartheta^+)$ and $B_\vartheta^+(z) = -(1 + \operatorname{cyc}\vartheta)^{1/2} + O(z - Z_\vartheta^+)$ are analytic functions of z. Furthermore the constants in the O-terms are uniform in ϑ, since they vary continuously on the compact fundamental domain $[-\pi/2, 3\pi/2)$ of ϑ. Similar arguments give

$$C_\vartheta(z) = A_\vartheta^-(z) + B_\vartheta^-(z)(1 - z/Z_\vartheta^-)^{1/2},$$

where $A_\vartheta^-(z) = \operatorname{cyc}(\vartheta - \pi) + O(z - Z_\vartheta^-)$ and $B_\vartheta^+(z) = -\big(1 + \operatorname{cyc}(\vartheta - \pi)\big)^{1/2} + O(z - Z_\vartheta^-)$ for the expansion of $C_\vartheta(z)$ in the neighbourhood of $z = Z_\vartheta^-$. These formulæ resolve the paradox mentioned above: the singularities of $C_\vartheta(z)$ "blink" at the cusps of the cycloid, where the factor multiplying $(1 - z/Z_\vartheta^\pm)^{1/2}$ vanishes. For the singularity at Z_ϑ^-, this occurs at $\vartheta = 0$, so that $R(z) = C_0(z)$ has just one singularity, at $z = Z_0 = Z_0^+$.

We now proceed, as indicated in the introduction, to extract the desired asymptotic information from $C_\vartheta(z)$. We define

$$R^*(z) = \frac{1}{2\pi} \int_{-\pi/2}^{3\pi/2} C_\vartheta(z)\, d\vartheta,$$

a power series in z in which the coefficients of odd powers of z vanish and the coefficient of the even power z^{2m} is the same as the coefficient of the term $x^m y^m$ in $R(x,y)$. Thus we have

$$\frac{R_{m,m}}{m!^2} = \frac{1}{2\pi} \int_{-\pi/2}^{3\pi/2} [z^{2m}]\, C_\vartheta(z)\, d\vartheta.$$

The largest contributions to this integral come from those ϑ for which the singularities of $C_\vartheta(z)$ are closest to the origin; for the singularity at Z_ϑ^+ this occurs for ϑ near 0, and for Z_ϑ^-, near π. Accordingly, we set

$$\varepsilon(n) = \left(\frac{48 \log n}{n}\right)^{1/2},$$

and break the interval $I = [-\pi/2, 3\pi/2)$ into three parts: $J^+ = [-\varepsilon(n), \varepsilon(n)]$, $J^- = [\pi - \varepsilon(n), \pi + \varepsilon(n)]$ and $K = I \setminus (J^+ \cup J^-)$.

First we consider the integral over ϑ in K. We have $Z_\vartheta^+ = \exp -\mathrm{cyc}\,\vartheta = \exp -\big(1 - \vartheta^2/8 + O(\vartheta^4)\big)$. Thus for ϑ not in J^+, we have $Z_\vartheta^+ \geq r$, where $r = \exp -\big(1 - \varepsilon(n)^2/16\big) = \exp -\big(1 - 3\log n/n\big)$. Similarly, for ϑ not in J^-, we have $Z_\vartheta^- \leq -r$. Thus for ϑ in K, $C_\vartheta(z)$ is analytic throughout the disk of radius r centred at the origin. By Cauchy's theorem, we have

$$\begin{aligned}[z^n]C_\vartheta(z) &= \frac{1}{2\pi i}\oint \frac{C_\vartheta(z)\,d\vartheta}{z^{n+1}}\\ &= O\left(\frac{1}{r^n}\right)\\ &= O\left(\frac{e^n}{n^3}\right),\end{aligned}$$

where the countour integral is taken in the positive sense around the circle of radius r centred at the origin. Thus we have

$$\frac{1}{2\pi}\int_K [z^n]C_\vartheta(z)\,d\vartheta = O\left(\frac{e^n}{n^3}\right).$$

For ϑ in J^+, we have by Darboux's lemma

$$\begin{aligned}[z^n]C_\vartheta(z) &= -(1+\mathrm{cyc}\,\vartheta)^{1/2}\binom{n-3/2}{n}\left(\frac{1}{Z_\vartheta^+}\right)^n + O\left(\binom{n-5/2}{n}\left(\frac{1}{Z_\vartheta^+}\right)^n\right)\\ &= \frac{e^n}{(2\pi)^{1/2}n^{3/2}}\left(1+O\left(\frac{(\log n)^2}{n}\right)\right)\exp -(n\vartheta^2/8),\end{aligned}$$

where we have estimated the leading factor by

$$-(1+\mathrm{cyc}\,\vartheta)^{1/2} = -\big(2+O(\vartheta^2)\big)^{1/2} = -2^{1/2}\big(1+O\big(\varepsilon(n)^2\big)\big) = -2^{1/2}\left(1+O\left(\frac{\log n}{n}\right)\right),$$

the singular point by

$$\begin{aligned}Z_\vartheta^+ &= \exp -\mathrm{cyc}\,\vartheta = \exp -\big(1-\vartheta^2/8+O(\vartheta^4)\big)\\ &= \exp -(1-\vartheta^2/8)\big(1+O\big(\varepsilon(n)^4\big)\big) = \exp -(1-\vartheta^2/8)\left(1+O\left(\left(\frac{\log n}{n}\right)^2\right)\right),\end{aligned}$$

and the binomial coefficients by

$$\binom{n-3/2}{n} = -\frac{1}{2\pi^{1/2}n^{3/2}}\left(1+O\left(\frac{1}{n}\right)\right)$$

and

$$\binom{n-5/2}{n} = O\left(\frac{1}{n^{5/2}}\right).$$

Thus we have

$$\begin{aligned}
&\frac{1}{2\pi}\int_{J+}[z^n]C_\vartheta(z)\,d\vartheta \\
&\qquad = \frac{e^n}{(2\pi)^{1/2}\,n^{3/2}}\left(1+O\left(\frac{(\log n)^2}{n}\right)\right)\int_{-\varepsilon(n)}^{\varepsilon(n)}\exp-(n\vartheta^2/8)\,d\vartheta \\
&\qquad = \frac{e^n}{\pi n^2}\left(1+O\left(\frac{(\log n)^2}{n}\right)\right),
\end{aligned}$$

where we have evaluated the integral by making the change of variable $\vartheta = 2\xi/n^{1/2}$ to obtain

$$\begin{aligned}
\exp-(n\vartheta^2/8)\,d\vartheta &= \frac{2}{n^{1/2}}\int_{-\delta(n)}^{\delta(n)}\exp-(\xi^2/2)\,d\xi \\
&= \frac{2}{n^{1/2}}\int_{-\infty}^{\infty}\exp-(\xi^2/2)\,d\xi \\
&\quad - \frac{2}{n^{1/2}}\int_{-\infty}^{-\delta(n)}\exp-(\xi^2/2)\,d\xi \\
&\quad - \frac{2}{n^{1/2}}\int_{\delta(n)}^{\infty}\exp-(\xi^2/2)\,d\xi \\
&= \frac{2^{3/2}\pi^{1/2}}{n^{1/2}} + O\left(\frac{1}{n^{12}(\log n)^{1/2}}\right),
\end{aligned}$$

where $\delta(n) = (24\log n)^{1/2}$.

For ϑ in J^-, similar arguments yield

$$\frac{1}{2\pi}\int_{J+}[z^n]C_\vartheta(z)\,d\vartheta = \pm\frac{e^n}{\pi n^2}\left(1+O\left(\frac{(\log n)^2}{n}\right)\right),$$

where the plus sign is taken for n even and the minus sign for n odd. (The alternation of sign arises from the negative branch point Z_ϑ^- being raised to the power n.) Combining these estimates, we conclude that

$$[z^n]R^*(z) = \frac{2e^n}{\pi n^2}\left(1+O\left(\frac{(\log n)^2}{n}\right)\right)$$

for even n. For odd n we know that $[z^n]R^*(z) = 0$, though this asymptotic analysis only yields $[z^n]R^*(z) = O\big(e^n(\log n)^2/n^3\big)$. Since $R_{m,m} = m!^2[z^{2m}]R^*(z)$ and $m!^2 = 2\pi m^{2m+1}e^{-2m}\big(1+O(1/m)\big)$, we conclude that $R_{m,m} = m^{2m-1}\big(1+O(1/m)\big)$, which is consistent with the exact result cited above. We observe that the limiting value, as n tends to infinity through even values, of the ratio of R_n^*/R_n (the probability that a randomly

chosen n-vertex labelled tree is equicolourable) to $\binom{n}{n/2}/2^n \sim (2/\pi n)^{1/2}$ (the probability that n vertices, independently assigned colours by unbiased coin flips, are equicoloured) is 2.

3. Rooted Trees

The problem of enumerating rooted unlabelled trees was first broached by Cayley [C1] in 1857. The problem is to determine the number r_n of different rooted trees on n vertices, where two trees are to be considered the same if there is an isomorphism between them (that is, a one-to-one correspondence between the vertices that preserves the root as well as the adjacency relation). Cayley did not quite give either a recurrence or a functional equation for the generating function for these trees, but rather gave a curious amalgam of the two that allows the number of rooted trees to be calculated expeditiously.

It was Pólya [P1,P2] who in 1937 first gave an enumeration of rooted trees entirely in terms of the generating function

$$r(z) = \sum_{n \geq 1} r_n \, z^n,$$

and it is his path that we shall follow and extend in our work. Note that, as is customary when enumerating unlabelled objects, $r(z)$ is an "ordinary," rather than an "exponential," generating function.

Pólya's first step was to formulate a component principle analogous to (2.1) for ordinary generating functions enumerating unlabelled objects. This principle states that if $f(z)$ is the ordinary generating function for unlabelled components, then

$$g(z) = \exp \sum_{h \geq 1} \frac{f(z^h)}{h} \tag{3.1}$$

is the ordinary generating function for unlabelled structures comprising zero or more disjoint components. Since a rooted tree comprises a root together with zero or more disjoint rooted trees (the subtrees adjacent to the root), $r(z)$ satisfies the functional equation

$$r(z) = z \exp \sum_{h \geq 1} \frac{r(z^h)}{h}. \tag{3.2}$$

Note that this functional equation is "non-local," in that the right-hand side involves the evaluation of r not only at z, but at its powers $z^2, z^3, \ldots$ as well.

That the asymptotic methods used for labelled trees in Section 2 (based on Darboux's lemma) can also be applied to (3.2) was indicated by Pólya, and carried out explicitly by Otter [O]. The first step is to find the singularity of $r(z)$ that is closest to the origin; this corresponds to the radius of convergence z_0 of $r(z)$. Since an unlabelled rooted tree on n vertices corresponds has at most $n!$ different labellings, the coefficients of $r(z)$ are greater than or equal to the corresponding coefficients of $R(z)$, and thus $z_0 \le Z_0 = 1/e$. On the other hand, each unlabelled rooted tree corresponds to at least one unlabelled ordered rooted tree (in which the offspring of each vertex are linearly ordered). The latter were enumerated by Cayley [C2], who showed that the number of such trees with n vertices is $\frac{1}{n}\binom{2n-2}{n-1} \le 4^{n-1}$. Thus the coefficients of $r(z)$ are less than the corresponding coefficients of $z/(1-4z)$, so that $z_0 \ge 1/4$.

To find the singularity z_0 more precisely, we write (3.2) as $\Phi\big(z, r(z)\big) = 0$, where

$$\Phi(z,w) = z \exp\big(w + \Psi(z)\big) - w$$

and

$$\Psi(z) = \sum_{h \ge 2} \frac{r(z^h)}{h}.$$

We observe that since $r(z)$ is analytic for z in the disk of radius $1/4$ centred at the origin, $\Psi(z)$, and thus also $\Phi(z,w)$, is analytic for z in the disk of radius $(1/4)^{1/2} = 1/2 > 1/e \ge z_0$ centred at the origin. To locate the singularity, we calculate

$$\frac{\partial}{\partial w}\Phi(z,w) = \Phi(z,w) + w - 1.$$

The singularity occurs when this derivative and $\Phi(z,w)$ vanish simulataneously for $w = r(z)$. This happens only for $w = w_0 = r(z_0) = 1$. Thus z_0 satisfies the equation

$$z_0 = \exp -\big(1 + \Psi(z_0)\big).$$

To determine the numerical value $z_0 = 0.3383\ldots$, we use the formula

$$\begin{aligned}\Psi(z) &= \sum_{h \ge 2} \frac{1}{h} \sum_{n \ge 1} r_n \, z^{nh} \\ &= \sum_{n \ge 1} r_n \left(\log \frac{1}{1 - z^n} - z^n \right),\end{aligned}$$

together with the coefficients r_n of the series $r(z)$, which can be calculated recursively from (3.2) (see Table 1).

To expand $r(z)$ in the neighbourhood of $z = z_0$, we calculate

$$\frac{\partial^2}{\partial w^2}\Phi(z,w) = \frac{\partial}{\partial w}\Phi(z,w) + 1 = \Phi(z,w) + w \tag{3.2$'$}$$

and

$$\frac{\partial}{\partial z}\Phi(z,w) = \big(\Phi(z,w) + w\big)\big(1 + z\Psi'(z)\big)/z. \tag{3.2$''$}$$

Then we have

$$\frac{\partial^2}{\partial w^2}\Phi(z,w)\big|_{w=w_0,z=z_0} = 1$$

and

$$\frac{\partial}{\partial z}\Phi(z,w)\big|_{w=w_0,z=z_0} = \big(1 + z_0\Psi'(z_0)\big)/z_0,$$

so that

$$\begin{aligned}\Phi(z,w) = \frac{1}{2}(w-w_0)^2 + O\big((w-w_0)^3\big)& \\ - A\,(1 - z/z_0) + O\big((w-w_0)(1-z/z_0)\big) + O\big((1-z/z_0)^2\big),&\end{aligned}$$

where $A = 1 + z_0\Psi'(z_0)$. To determine the numerical value $A = 1.215\ldots$, we use the formula

$$\begin{aligned} z\Psi'(z) &= \sum_{h\geq 2}\sum_{n\geq 1} n r_n\, z^{nh} \\ &= \sum_{n\geq 1} n r_n \left(\frac{z^n}{1-z^n} - z^n\right). \end{aligned}$$

Thus at $z = z_0$, $r(z)$ has a branch point of order 2, and an expansion of the form

$$r(z) = a(z) + b(z)(1 - z/z_0)^{1/2}$$

where $a(z) = 1 + O(z - z_0)$ and $b(z) = -(2A)^{1/2} + O(z - z_0)$ are analytic functions of z. Applying Darboux's lemma, we conclude that $[z^n]r(z)$ is asymptotic to $A^{1/2} z_0^{-n}/n^{3/2}(2\pi)^{1/2}$, where $(A/2\pi)^{1/2} = 0.4399\ldots$.

We now turn to the problem of enumerating equicolourable unlabelled rooted trees. Let $r_{l,m}$ denote the number of red-rooted unlabelled trees with $l \geq 1$ red vertices and $m \geq 0$ blue vertices. Let

$$r(x,y) = \sum_{l\geq 1, m\geq 0} r_{l,m}\, x^l y^m$$

be the bivariate ordinary generating function for red-rooted unlabelled trees. The component principle analogous to (3.1) for bivariate ordinary generating functions is

$$g(x,y) = \exp \sum_{h\geq 1} \frac{f(x^h, y^h)}{h},$$

where $f(x,y)$ is the generating function for components and $g(x,y)$ is the generating function for structures comprising zero or more disjoint components. Since a red-rooted tree comprises a red root (enumerated by x) together with zero or more disjoint blue-rooted trees (enumerated by $r(y,x)$), $r(x,y)$ satisfies the functional equation

$$r(x,y) = x \exp \sum_{h\geq 1} \frac{r(y^h, x^h)}{h}. \tag{3.3}$$

We shall derive from this functional equation the asymptotic behaviour of the coefficients $r_{m,m}$.

We begin by making the substitutions $x = z\exp(i\vartheta)$ and $y = z\exp(-i\vartheta)$, and thus defining

$$r_\vartheta(z) = r\big(z\exp(i\vartheta), z\exp(-i\vartheta)\big). \tag{3.4}$$

From (3.3) and (3.4) we obtain

$$r_\vartheta(z) = z\exp\left(i\vartheta + \sum_{h\geq 1} \frac{r_{-h\vartheta}(z^h)}{h}\right) \tag{3.5}$$

as the functional equation satisfied by $r_\vartheta(z)$.

As before, it will be convenient to work with relatives of $r_\vartheta(z)$ that are real when ϑ and z are real. Thus we define

$$c_\vartheta(z) = \frac{r_\vartheta(z) + r_{-\vartheta}(z)}{2} \tag{3.6}$$

and

$$s_\vartheta(z) = \frac{r_\vartheta(z) - r_{-\vartheta}(z)}{2i}. \tag{3.7}$$

We can find the functional equations satisfied by $c_\vartheta(z)$ and $s_\vartheta(z)$ by substituting (3.5) into (3.6) and (3.7), then substituting $r_\vartheta(z) = c_\vartheta(z) + i\,s_\vartheta(z)$ and $r_{-\vartheta(z)} = c_\vartheta(z) - i\,s_\vartheta(z)$ into the result, to obtain

$$c_\vartheta(z) = z\exp\left(\sum_{h\geq 1} \frac{c_{h\vartheta}(z^h)}{h}\right)\cos\left(\vartheta - \sum_{h\geq 1} \frac{s_{h\vartheta}(z^h)}{h}\right) \tag{3.8}$$

and

$$s_\vartheta(z) = z \exp\left(\sum_{h\geq 1} \frac{c_{h\vartheta}(z^h)}{h}\right) \sin\left(\vartheta - \sum_{h\geq 1} \frac{s_{h\vartheta}(z^h)}{h}\right). \tag{3.9}$$

To determine the singularities of $c_\vartheta(z)$ as a function of z with ϑ fixed, we eliminate $s_\vartheta(z)$ from (3.8) and (3.9). Squaring and adding these equations, we obtain

$$c_\vartheta(z)^2 + s_\vartheta(z)^2 = z^2 \exp\bigl(2c_\vartheta(z) + 2\Psi_\vartheta(z)\bigr),$$

where

$$\Psi_\vartheta(z) = \sum_{h\geq 2} \frac{c_{h\vartheta}(z^h)}{h}.$$

This result allows us to eliminate $s_\vartheta(z)$ from (3.8), obtaining

$$c_\vartheta(z) = z \exp\bigl(c_\vartheta(z) + \Psi_\vartheta(z)\bigr) \cos\left(\vartheta - \bigl(z^2 \exp\bigl(2c_\vartheta(z) + 2\Psi_\vartheta(z)\bigr) - c_\vartheta(z)^2\bigr)^{1/2} - \Upsilon_\vartheta(z)\right),$$

where

$$\Upsilon_\vartheta(z) = \sum_{h\geq 2} \frac{s_{h\vartheta}(z^h)}{h}.$$

This equation can be written as $\Phi_\vartheta\bigl(z, c_\vartheta(z)\bigr) = 0$, where

$$\Phi_\vartheta(z,w) = z \exp\bigl(w + \Psi_\vartheta(z)\bigr) \cos\left(\vartheta - \bigl(z^2 \exp\bigl(2w + 2\Psi_\vartheta(z)\bigr) - w^2\bigr)^{1/2} - \Upsilon_\vartheta(z)\right) - w.$$

To locate the singularities of $c_\vartheta(z)$, we calculate

$$\frac{\partial}{\partial w}\Phi_\vartheta(z,w) = \Phi_\vartheta(z,w) - 1 + z^2 \exp\bigl(2w + 2\Psi_\vartheta(z)\bigr).$$

The singularities occur when this derivative and $\Phi_\vartheta(z,w)$ vanish simultaneously for $z = z_\vartheta^\pm$ and $w = c_\vartheta(z_\vartheta^\pm)$, so that we have

$$z_\vartheta^\pm = \pm \exp -\bigl(c_\vartheta(z_\vartheta^\pm) + \Psi_\vartheta(z_\vartheta^\pm)\bigr). \tag{3.10}$$

Substituting this relation into (3.8) and (3.9) yields

$$c_\vartheta(z_\vartheta^\pm) = \pm \cos\bigl(\vartheta - s_\vartheta(z_\vartheta^\pm) - \Upsilon_\vartheta(z_\vartheta^\pm)\bigr),$$

and

$$s_\vartheta(z_\vartheta^\pm) = \pm \sin\bigl(\vartheta - s_\vartheta(z_\vartheta^\pm) - \Upsilon_\vartheta(z_\vartheta^\pm)\bigr),$$

where of course we must take the same sign throughout all three equations. We can again express the solutions to these equations in terms of the cycloid function:

$$z_\vartheta^+ = \exp -\big(\mathrm{cyc}\big(\vartheta - \Upsilon_\vartheta(z_\vartheta^+)\big) + \Psi_\vartheta(z_\vartheta^+)\big) \tag{3.11}$$

and

$$z_\vartheta^- = -\exp -\big(\mathrm{cyc}\big(\vartheta - \pi - \Upsilon_\vartheta(z_\vartheta^-)\big) + \Psi_\vartheta(z_\vartheta^-)\big).$$

To expand $c_\vartheta(z)$ in the neighbourhood of $z = z_\vartheta^+$, we calculate

$$\begin{aligned}\frac{\partial^2}{\partial w^2}\Phi_\vartheta(z,w) &= \frac{\partial}{\partial w}\Phi_\vartheta(z,w) + 2z^2\exp\big(2w + 2\Psi_\vartheta(z)\big)\\ &= \Phi_\vartheta(z,w) - 1 + 3z^2\exp\big(2w + 2\Psi_\vartheta(z)\big)\end{aligned}$$

and

$$\begin{aligned}\frac{\partial}{\partial z}\Phi_\vartheta(z,w) = {}& \big(\Phi_\vartheta(z,w) + w\big)\big(1 + z\Psi'_\vartheta(z)\big)/z\\ &+ z^2\exp\big(3w + 3\Psi_\vartheta(z)\big)\,\big(1 + z\Psi'_\vartheta(z)\big)\\ &+ z\exp\big(w + \Psi_\vartheta(z)\big)\,\big(z^2\exp\big(2w + 2\Psi_\vartheta(z)\big) - w^2\big)^{1/2}\;\Upsilon'_\vartheta(z).\end{aligned}$$

Then we have

$$\frac{\partial^2}{\partial w^2}\Phi_\vartheta(z,w)\big|_{w=w_\vartheta^+, z=z_\vartheta^+} = 2$$

and

$$\frac{\partial}{\partial z}\Phi_\vartheta(z,w)\big|_{w=w_\vartheta^+, z=z_\vartheta^+} = \frac{(1+w_\vartheta^+)\big(1 + z_\vartheta^+\Psi'(z_\vartheta^+)\big) + \big(1-(w_\vartheta^+)^2\big)^{1/2}\,z_\vartheta^+\Upsilon'_\vartheta(z_\vartheta^+)}{z_\vartheta^+},$$

so that

$$\begin{aligned}\Phi_\vartheta(z,w) = {}& (w - w_\vartheta^+)^2 + O\big((w-w_\vartheta^+)^3\big)\\ &- A_\vartheta^+\,(1 - z/z_\vartheta^+) + O\big((w-w_\vartheta^+)(1-z/z_\vartheta^+)\big) + O\big((1-z/z_\vartheta^+)^2\big),\end{aligned}$$

where

$$\begin{aligned}A_\vartheta^+ &= (1+w_\vartheta^+)\big(1 + z_\vartheta^+\Psi'(z_\vartheta^+)\big) + \big(1-(w_\vartheta^+)^2\big)^{1/2}\,z_\vartheta^+\Upsilon'_\vartheta(z_\vartheta^+)\\ &= \big(1 + \mathrm{cyc}\big(\vartheta - \Upsilon_\vartheta(z_\vartheta^+)\big)\big)\big(1 + z_\vartheta^+\Psi'(z_\vartheta^+)\big) + \mathrm{cocyc}\big(\vartheta - \Upsilon_\vartheta(z_\vartheta^+)\big)\,z_\vartheta^+\Upsilon'_\vartheta(z_\vartheta^+).\end{aligned}$$

Thus at $z = z_\vartheta^+$, $c_\vartheta(z)$ has a branch point of order 2 and, in the neighbourhood of $z = z_\vartheta^+$, an expansion of the form

$$c_\vartheta^+(z) = a_\vartheta^+(z) + b_\vartheta^+(z)(1 - z/z_\vartheta^+)^{1/2},$$

where $a_\vartheta^+(z) = \mathrm{cyc}\big(\vartheta - \Upsilon_\vartheta(z_\vartheta^+)\big) + O(z - z_\vartheta^+)$ and $b_\vartheta^+(z) = -(A_\vartheta^+)^{1/2} + O(z - z_\vartheta^+)$ are analytic functions of z, and where again the constants in the O-terms are uniform in ϑ. Similar arguments give, in the neighbourhood of $z = z_\vartheta^-$, an expansion of the form

$$c_\vartheta^-(z) = a_\vartheta^-(z) + b_\vartheta^-(z)(1 - z/z_\vartheta^-)^{1/2},$$

where $a_\vartheta^-(z) = \mathrm{cyc}\big(\vartheta - \pi - \Upsilon_\vartheta(z_\vartheta^-)\big) + O(z - z_\vartheta^-)$, $b_\vartheta^-(z) = -(A_\vartheta^-)^{1/2} + O(z - z_\vartheta^-)$ and

$$\begin{aligned} A_\vartheta^- &= (-1 + w_\vartheta^-)\big(1 + z_\vartheta^- \Psi'(z_\vartheta^-)\big) - \big(1 - (w_\vartheta^-)^2\big)^{1/2} z_\vartheta^- \Upsilon'_\vartheta(z_\vartheta^-) \\ &= \big(-1 + \mathrm{cyc}\big(\vartheta - \pi - \Upsilon_\vartheta(z_\vartheta^-)\big)\big)\big(1 + z_\vartheta^- \Psi'(z_\vartheta^-)\big) - \mathrm{cocyc}\big(\vartheta - \pi - \Upsilon_\vartheta(z_\vartheta^-)\big)\, z_\vartheta^- \Upsilon'_\vartheta(z_\vartheta^-). \end{aligned}$$

We are now ready to extract the desired asymptotic information from these expansions for $c_\vartheta(z)$. We define

$$r^*(z) = \frac{1}{2\pi} \int_{-\pi/2}^{3\pi/2} c_\vartheta(z)\, d\vartheta,$$

a power series in z in which the coefficients of odd powers of z vanish and the coefficient of the even power z^{2m} is the same as the coefficient of the term $x^m y^m$ in $r(x, y)$. Thus we have

$$r_{m,m} = \frac{1}{2\pi} \int_{-\pi/2}^{3\pi/2} [z^{2m}]\, c_\vartheta(z)\, d\vartheta. \tag{3.12}$$

The estimation of this integral is completely analogous to that in the preceding section. The only differences are in the locations of the singularities $z_\vartheta^\pm$, and in the constant terms of the functions $a_\vartheta^\pm$ and $b_\vartheta^\pm$. Furthermore, these values affect the leading term of the asymptotics only through their dependence on ϑ in the neighbourhoods of $\vartheta = 0$ (for the plus superscript) and $\vartheta = \pi$ (for the minus superscript). We begin with the plus superscript. Simple arguments show that z_ϑ^+ is an even analytic function of ϑ, and $z_0^+ = z_0$, as in the univariate case. Thus in the neighbourhood of $\vartheta = 0$ we have

$$z_\vartheta^+ = z_0 \left(1 + \frac{\ddot{z}_0^+}{2 z_0}\, \vartheta^2 + O(\vartheta^4)\right),$$

where dots indicate differentiation with respect to the subscript (as opposed to primes, which indicate differentiation with respect to a parenthesized argument). To determine $\ddot{z}_0^+$, we use the equation (3.11). For the cycloid function, we have the expansion $\mathrm{cyc}\,\vartheta = 1 - \vartheta^2/8 + O(\vartheta^4)$ in the neighbourhood of $\vartheta = 0$. The function $\Upsilon_\vartheta(z)$ is an odd analytic function of ϑ, so we have $\Upsilon_\vartheta(z_\vartheta^+) = \dot{\Upsilon}_0(z_0^+)\vartheta + O(\vartheta^3)$ in the neighbourhood of $\vartheta = 0$. And the function $\Psi_\vartheta(z)$ is an even analytic function of ϑ, so we have $\Psi_\vartheta(z_\vartheta^+) = \Psi_0(z_0^+) + \big(\ddot{\Psi}_0(z_0^+) + \Psi'_0(z_0^+)\, \ddot{z}_0^+\big)\vartheta^2/2 + O(\vartheta^4)$ in the neighbourhood of $\vartheta = 0$. Combining these results

with (3.11) yields $\ddot{z}_0^+/2z_0 = (B^2 - 4C)/8A$, where $B = 1 - \dot{\Upsilon}_0(z_0^+)$ and $C = \ddot{\Psi}_0(z_0^+)$, so that

$$z_\vartheta^+ = z_0 \left(1 + \frac{B^2 - 4C}{8A}\,\vartheta^2 + O(\vartheta^4)\right).$$

The constant terms of $a_\vartheta^+(z) = 1 + O(\vartheta^2) + O(z - z_\vartheta^+)$ and $b_\vartheta^+(z) = -(2A)^{1/2} + O(\vartheta^2) + O(z - z_\vartheta^+)$ are the same as in the univariate case. For the minus superscript, similar calculations yield

$$z_\vartheta^- = z_0 \left(1 + \frac{B^2 - 4C}{8A}\,\vartheta^2 + O(\vartheta^4)\right),$$

$a_\vartheta^-(z) = 1 + O(\vartheta^2) + O(z - z_\vartheta^-)$ and $b_\vartheta^-(z) = -(2A)^{1/2} + O(\vartheta^2) + O(z - z_\vartheta^-)$. With these expansions, we can estimate (3.12) as in the preceding section to obtain

$$[z^n]r^*(z) = \frac{2A\, z_0^{-n}}{\pi(B^2 - 4C)^{1/2}\, n^2}\left(1 + O\left(\frac{(\log n)^2}{n}\right)\right) \tag{3.13}$$

for even n. For odd n we know that $[z^n]r^*(z) = 0$.

It remains to determine the numerical values of the constants in (3.13). For B, we start with

$$\dot{s}_0(z) = \sum_{l\ge 1, m\ge 0} (l - m) r_{l,m}\, z^{l+m} = q(z),$$

where

$$q(z) = \left(\left(x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y}\right) r(x,y)\right)\Bigg|_{x=z,\,y=z}.$$

The coefficients of the series $q(z) = \sum_{n\ge 1} q_n\, z^n$ can be calculated from the coefficients $r_{l,m}$, which can in turn be calculated recursively from (3.3) (see Table 1). To determine the numerical value $B = 1 - \dot{\Upsilon}_0(z_0) = 0.8269\ldots$, we use the formula

$$\begin{aligned}
\dot{\Upsilon}_0(z) &= \sum_{h\ge 2} \dot{s}_0(z) \\
&= \sum_{h\ge 2}\sum_{n\ge 1} q_n\, z^{nh} \\
&= \sum_{n\ge 1} q_n \left(\frac{z^n}{1 - z^n} - z^n\right).
\end{aligned}$$

For C, we start with

$$\ddot{c}_0(z) = -\sum_{l\ge 1, m\ge 0} (l - m)^2 r_{l,m}\, z^{l+m} = -p(z),$$

where

$$p(z) = \left(\left(x\frac{\partial}{\partial x} - y\frac{\partial}{\partial y} \right)^2 r(x,y) \right) \Big|_{x=z,y=z}.$$

The coefficients of the series $p(z) = \sum_{n\geq 1} p_n z^n$ can also be calculated from the coefficients $r_{l,m}$ (see Table 1). To determine the numerical value $C = \ddot{\Psi}_0(z_0) = -0.4450\ldots$, we use the formula

$$\begin{aligned} \ddot{\Psi}_0(z) &= \sum_{h\geq 2} h\, \ddot{c}_0(z) \\ &= -\sum_{h\geq 2} h \sum_{n\geq 1} p_n\, z^{nh} \\ &= -\sum_{n\geq 1} p_n \left(\frac{z^n}{(1-z^n)^2} - z^n \right). \end{aligned}$$

Combining these results gives $2A/\pi(B^2 - 4C)^{1/2} = 0.4931\ldots$ for the constant appearing in (3.13). We observe that the limiting value, as n tends to infinity through even values, of the ratio of r_n^*/r_n (the probability that a randomly chosen n-vertex rooted tree is equicolourable) to $\binom{n}{n/2}/2^n \sim (2/\pi n)^{1/2}$ (the probability that n vertices, independently assigned colours by unbiased coin flips, are equicoloured) is $2A^{1/2}/(B^2 - 4C)^{1/2} = 1.40499\ldots$.

n	r_n	q_n	p_n	r_n^*
1	1	1	1	0
2	1	0	0	1
3	2	0	2	0
4	4	0	8	2
5	9	1	25	0
6	20	2	68	9
7	48	8	192	0
8	115	18	516	44
9	286	52	1438	0
10	719	130	3964	249
11	1842	348	11098	0
12	4766	904	31056	1506
13	12486	2416	87694	0
14	32973	6404	247960	9687
15	87811	17213	704571	0

Table 1. Coefficients in the series $r(z)$, $q(z)$, $p(z)$ and $r^*(z)$.

4. Unrooted Trees

The enumeration of unrooted unlabelled trees was first undertaken by Cayley, who in 1875 [C3] gave it in terms of a two-parameter enumeration of rooted trees by size and depth. In 1881 [C4], he expressed the numbers u_n of unrooted trees exclusively in terms of the numbers r_n of rooted trees. In 1948, Otter [O] expressed the generating function

$$u(z) = \sum_{n \geq 1} u_n \, z^n$$

for unrooted trees in terms of the generating function

$$r(z) = \sum_{n \geq 1} r_n \, z^n$$

for rooted trees,

$$u(z) = r(z) - \frac{1}{2} r(z)^2 + \frac{1}{2} r(z^2), \tag{4.1}$$

and from this he was able to deduce the asymptotic behaviour,

$$u_n \sim \frac{A^{3/2}}{(2\pi)^{1/2}} \, \frac{z_0^{-n}}{n^{5/2}}, \tag{4.2}$$

where $A = 1.215\ldots$ and $z_0 = 0.3383\ldots$ are as defined in Section 3.

If T is an unrooted tree, let v_T denote the number of orbits of its vertices under the action of its automorphism group, let e_T denote the number of orbits of edges, and let s_T denote 1 or 0 according as T is or is not *edge-symmetric*; that is, according as there is or is not an automorphism of T that exchanges the vertices of some edge of T. Otter established the identity

$$1 = v_T - e_T + s_T. \tag{4.3}$$

If n_T denotes the number of vertices in T, then multiplying (4.3) by z^{n_T} and summing over all unrooted trees T yields for the left-hand side the generating function $u(z)$ for unrooted trees. Since the unrooted tree T can be rooted in v_T different ways, the sum of $v_T \, z^{n_T}$ yields $r(z)$. Similarly, the sum of $e_T \, z^{n_T}$ yields the generating function for trees rooted at an edge rather than a vertex; this is easily seen to be $\frac{1}{2}\big(r(z)^2 + r(z^2)\big)$. Finally, the sum of $s_T \, z^{n_T}$ is the generating function for edge-symmetric trees; this is easily seen to be $\frac{1}{2} r(z^2)$. Combining these results yields Otter's identity (4.1).

To derive the asymptotic behaviour (4.2), we again apply Darboux's lemma to the singularity of $u(z)$ that is closest to the origin. This singularity is at z_0, and it arises from the contributions of $r(z)$ and $-\frac{1}{2} r(z)^2$. The term $\frac{1}{2} r(z^2)$ has no singularity closer

to the origin than $z_0^{1/2} > z_0$, and thus makes a negligible contribution to the asymptotic behaviour. With an eye to what is to come, we shall define the generating function $h(z) = \sum_{n\geq 1} h_n\, z^n$ by

$$h(z) = 2r(z) - r(z)^2\,, \tag{4.3$'$}$$

so that $u(z) = \frac{1}{2}h(z) + \frac{1}{2}r(z^2)$. We shall show that

$$h_n \sim \frac{2A^{3/2}}{(2\pi)^{1/2}}\,\frac{z_0^{-n}}{n^{5/2}}, \tag{4.3$''$}$$

which implies (4.2).

To expand $u(z)$ in the neighbourhood of $z = z_0$, we must extend the expansion of $r(z)$, obtained in Section 3, to higher terms. We have

$$r(z) = a(z) + b(z)(1 - z/z_0)^{1/2}, \tag{4.4}$$

where $a(z) = \sum_{k\geq 0} a_k\,(1 - z/z_0)^k$ and $b(z) = \sum_{k\geq 0} b_k\,(1 - z/z_0)^k$ are analytic at $z = z_0$. We have seen that $a_0 = 1$ and $b_0 = -(2A)^{1/2}$. We shall show now that $a_1 = 2A/3$.

Continuing from (3.2') we have

$$\frac{\partial^3}{\partial w^3}\Phi(z,w) = \frac{\partial}{\partial w}\Phi(z,w) + 1 = \Phi(z,w) + w,$$

so that

$$\frac{\partial^3}{\partial w^3}\Phi(z,w)\big|_{w=w_0,\,z=z_0} = 1.$$

Continuing from (3.2") we have

$$\frac{\partial^2}{\partial w\partial z}\Phi(z,w) = \big(\Phi(z,w) + w\big)\big(1 + z\,\Psi'(z)\big)/z,$$

so that

$$\frac{\partial^2}{\partial w\partial z}\Phi(z,w)\big|_{w=w_0,\,z=z_0} = \big(1 + z_0\Psi'(z_0)\big)/z_0.$$

Combining these results yields

$$\begin{aligned}\Phi(z,w) = \frac{1}{2}(w-w_0)^2 + \frac{1}{6}(w-w_0)^3 + O\big((w-w_0)^4\big)\\ - A\,(1 - z/z_0) - A\,(w-w_0)(1-z/z_0)\\ + O\big((w-w_0)^2(1-z/z_0)\big) + O\big((1-z/z_0)^2\big),\end{aligned}$$

where as before $A = 1 + z_0\Psi'(z_0)$. Since we have $\Phi\big(z, r(z)\big) = 0$, this expansion implies (4.4) with $a_0 = 1$, $b_0 = -(2A)^{1/2}$ and $a_1 = 2A/3$. Substituting this expansion into the right-hand side of (4.3') yields that

$$h(z) = f(z) + g(z)(1 - z/z_0)^{1/2},$$

where $f(z)$ and $g(z) = \sum_{k\geq 0} g_k\,(1 - z/z_0)^k$ are analytic at $z = z_0$, $g_0 = 0$ and $g_1 = 2(2A)^{3/2}/3$. Applying Darboux's lemma to the singularity of $h(z)$ at $z = z_0$ yields (4.3") and thus Otter's asymptotic formula (4.2).

To enumerate equicolourable unrooted trees, our first task is to find an analogue of Otter's identity (4.1). Let T be an unrooted tree. If one bicolouring of T has a_T red and b_T blue vertices, then the other bicolouring has b_T red and a_T blue vertices. Thus the polynomial $\frac{1}{2}(x^{a_T}\,y^{b_T} + x^{b_T}\,y^{a_T})$ depends only on T, and not on the particular bicolouring considered. We define

$$u(x, y) = \frac{1}{2}\sum_T x^{a_T}\,y^{b_T} + x^{b_T}\,y^{a_T},$$

where the sum is over all unrooted trees. Our goal is to establish the identity

$$u(x, y) = \frac{1}{2}r(x, y) + \frac{1}{2}r(y, x) - \frac{1}{2}r(x, y)\,r(y, x) + \frac{1}{2}r(xy), \tag{4.5}$$

analogous to (4.1).

Let S be a bicoloured unrooted tree, and let a_S and b_S denote the numbers of red and blue vertices, respectively, in S. We define

$$h(x, y) = \sum_S x^{a_S}\,y^{b_S},$$

where the sum is over all bicoloured unrooted trees. An unrooted tree has two distinct bicolourings unless it is edge-symmetric, in which case it has just one. This yields

$$u(x, y) = \frac{1}{2}h(x, y) + \frac{1}{2}r(xy),$$

since $r(xy)$ enumerates bicoloured edge-symmetric unrooted trees. Thus, to establish (4.5) it will suffice to show that

$$h(x, y) = r(x, y) + r(y, x) - r(x, y)\,r(y, x). \tag{4.6}$$

Again using the fact that an unrooted tree has one or two bicolourings according as it is or is not edge-symmetric, we have

$$h(x,y) = \frac{1}{2}\sum_T (2 - s_T)(x^{a_T}\, y^{b_T} + x^{b_T}\, y^{a_T}).$$

From (4.3) we have $2 - s_T = 2v_T - 2e_T + s_T$, so that

$$h(x,y) = \sum_T v_T\,(x^{a_T}\, y^{b_T} + x^{b_T}\, y^{a_T}) - \frac{1}{2}\sum_T (2e_T - s_T)(x^{a_T}\, y^{b_T} + x^{b_T}\, y^{a_T}). \tag{4.7}$$

Since an unrooted tree T can be rooted in v_T different ways, we have

$$\sum_T v_T\,(x^{a_T}\, y^{b_T} + x^{b_T}\, y^{a_T}) = r(x,y) + r(y,x).$$

Let d_T denote the number of different ways in which T can be rooted in a directed edge. Then $d_T = 2e_T - s_T$. Thus we have

$$\begin{aligned}\sum_T (2e_T - s_T)(x^{a_T}\, y^{b_T} + x^{b_T}\, y^{a_T}) &= \sum_T d_T\,(x^{a_T}\, y^{b_T} + x^{b_T}\, y^{a_T}) \\ &= 2r(x,y)\,r(y,x),\end{aligned}$$

since each directed-edge-rooted tree can be decomposed in a unique way into a red-rooted tree whose root is the source of a directed edge whose target is the root of a blue-rooted tree, or into a blue-rooted tree whose root is the source of a directed edge whose target is the root of a red-rooted tree. Substituting these results into (4.7) yields (4.6) and thus (4.5).

At this point we can express the generating functions $u^*(z) = \sum_{n\ge 1} u_n^*\, z^n$ and $h^*(z) = \sum_{n\ge 1} h_n^*\, z^n$ for equicolourable and equicoloured unrooted trees, respectively, as

$$u^*(z) = \frac{1}{4\pi}\int_{-\pi/2}^{3\pi/2} r_\vartheta(z) + r_{-\vartheta}(z) - r_\vartheta(z)\,r_{-\vartheta}(z) + r(z^2)\,d\vartheta \tag{4.8}$$

and

$$h^*(z) = \frac{1}{2\pi}\int_{-\pi/2}^{3\pi/2} r_\vartheta(z) + r_{-\vartheta}(z) - r_\vartheta(z)\,r_{-\vartheta}(z)\,d\vartheta. \tag{4.9}$$

The coefficients of these generating functions, together with those of $u(z) = \sum_{n\geq 1} u_n z^n$ for unrooted trees, are tabulated in Table 2.

n	u_n	u_n^*	h_n^*
1	1	0	0
2	1	1	1
3	1	0	0
4	2	1	1
5	3	0	0
6	6	3	4
7	11	0	0
8	23	9	14
9	47	0	0
10	106	37	65
11	235	0	0
12	551	168	316
13	1301	0	0
14	3159	895	1742
15	7741	0	0

Table 2. Coefficients in the series $u(z)$, $u^*(z)$ and $h^*(z)$.

To determine the asymptotic behaviour of the coefficients u_n^* and h_n^*, we shall apply Darboux's lemma to (4.8) and (4.9). It will suffice to deal with (4.9), since (4.8) differs merely by a factor of 2 and the additional term $r(z^2)$, which (having no singularity closer to the origin than $z_0^{1/2} > z_0$) makes an asymptotically negligible contribution. To deal with (4.9), we define $h_\vartheta(z)$ to be the integrand,

$$h_\vartheta(z) = r_\vartheta(z) + r_{-\vartheta}(z) - r_\vartheta(z)\, r_{-\vartheta}(z),$$

which (using (3.6) and (3.5)) we can rewrite as

$$h_\vartheta(z) = 2c_\vartheta(z) - z^2 \exp\bigl(2c_\vartheta(z) + 2\Psi_\vartheta(z)\bigr). \tag{4.10}$$

From (4.10), we see that the singularities of $h_\vartheta(z)$ closest to the origin are, just as for $c_\vartheta(z)$, at z_ϑ^+ and z_ϑ^-. Starting with the singularity at z_ϑ^+, we seek to expand $h_\vartheta(z)$ in a neighbourhood of z_ϑ^+ as

$$h_\vartheta^+(z) = f_\vartheta^+(z) + g_\vartheta^+(z)\,(1 - z/z_\vartheta^+)^{1/2},$$

where $f_\vartheta^+(z)$ and $g_\vartheta^+(z)$ are analytic at $z = z_\vartheta^+$. Let us expand $g_\vartheta^+(z)$ as $g_\vartheta^+(z) = \sum_{k\geq 0} g_{\vartheta,k}^+ (1 - z/z_\vartheta^+)^k$.

We shall show first that

$$g_{\vartheta,0}^+ = 0, \tag{4.11}$$

independently of ϑ. For the first term on the right-hand side of (4.10), we have

$$2c_\vartheta^+(z) = 2a_\vartheta^+(z) + 2b_\vartheta^+(z)(1 - z/z_\vartheta^+)^{1/2} \tag{4.12}$$

in a neighbourhood of z_ϑ^+. For the second term, we have

$$z^2 \exp\bigl(2c_\vartheta(z) + 2\Psi_\vartheta(z)\bigr) = z^2 \exp\bigl(2a_\vartheta^+(z) + 2b_\vartheta^+(z)(1 - z/z_\vartheta^+)^{1/2} + 2\Psi_\vartheta(z)\bigr).$$

By (3.10), this expression tends to 1 as z tends to z_ϑ^+. Since $\exp\bigl(2b_\vartheta^+(z)(1-z/z_\vartheta^+)^{1/2}\bigr)$ also tends to 1 in this limit, we conclude that $\exp\bigl(2a_\vartheta^+(z) + 2\Psi_\vartheta(z)\bigr)$ tends to 1 as z tends to z_ϑ^+. Since this last expression is analytic at z_ϑ^+, we have

$$\exp\bigl(2a_\vartheta^+(z) + 2\Psi_\vartheta(z)\bigr) = 1 + O(1 - z/z_\vartheta^+).$$

We also have

$$\exp\bigl(2b_\vartheta^+(z)(1 - z/z_\vartheta^+)^{1/2}\bigr) = 1 + 2b_\vartheta^+(z)(1 - z/z_\vartheta^+)^{1/2} + O(1 - z/z_\vartheta^+),$$

we conclude that

$$z^2 \exp\bigl(2c_\vartheta(z) + 2\Psi_\vartheta(z)\bigr) = 1 + 2b_\vartheta^+(z)(1 - z/z_\vartheta^+)^{1/2} + O(1 - z/z_\vartheta^+).$$

Combining this with (4.12) in (4.10) yields $g_\vartheta^+(z) = O(1 - z/z_\vartheta^+)$, which is (4.11).

Since $g_{\vartheta,1}^+$ is an even analytic function of ϑ, we have

$$g_{\vartheta,1}^+ = g_{0,1}^+ + O(\vartheta^2).$$

To determine the value of $g_{0,1}^+$, we observe that $g_0^+(z) = g(z)$, so that $g_{0,1}^+ = g_1 = 2(2A)^{3/2}/3$. Thus we have

$$g_{\vartheta,1}^+ = \frac{2}{3}(2A)^{3/2} + O(\vartheta^2).$$

Combining this with (4.11) yields

$$g_\vartheta^+(z) = \frac{2}{3}(2A)^{3/2}(1 - z/z_\vartheta^+) + O\bigl(\vartheta^2(1 - z/z_\vartheta^+)\bigr) + O\bigl((1 - z/z_\vartheta^+)^2\bigr).$$

Similar arguments give, in the neighbourhood of $z = z_\vartheta^-$, an expansion of the form

$$h_\vartheta^-(z) = f_\vartheta^-(z) + g_\vartheta^-(z)\,(1 - z/z_\vartheta^-)^{1/2},$$

where

$$g_\vartheta^-(z) = \frac{2}{3}(2A)^{3/2}(1 - z/z_\vartheta^-) + O\big(\vartheta^2(1 - z/z_\vartheta^-)\big) + O\big((1 - z/z_\vartheta^-)^2\big).$$

With these expansions for the singularities of $h_\vartheta(z)$, we can proceed as before to apply Darboux's lemma to the integrand for each value of ϑ, then integrate the result from $-\pi/2$ to $3\pi/2$, with the greatest contributions coming when ϑ is near 0 or π. For even n the results are

$$h_n^* \sim \frac{4A^2}{\pi(B^2 - 4C)^{1/2}}\,\frac{z_0^{-n}}{n^3}$$

for (4.9) and

$$u_n^* \sim \frac{2A^2}{\pi(B^2 - 4C)^{1/2}}\,\frac{z_0^{-n}}{n^3}$$

for (4.8). For n odd, of course, $h_n^* = u_n^* = 0$. We observe that the limiting value, as n tends to infinity through even values, of the ratio of u_n^*/u_n (the probability that a randomly chosen n-vertex unrooted tree is equicolourable) to $\binom{n}{n/2}/2^n \sim (2/\pi n)^{1/2}$ (the probability that n vertices, independently assigned colours by unbiased coin flips, are equicoloured) is $2A^{1/2}/(B^2 - 4C)^{1/2} = 1.40499\ldots$.

5. Conclusion

All of our results enumerating equicolourable trees have been obtained by first enumerating equicoloured trees, then relying on a relatively simple relationship between the two enumerations. We conclude by mentioning some problems where the relationship is more complicated. First, we may consider the enumeration of equicolourable forests (wherein the individual trees need not be equicolourable). It should be relatively easy to enumerate equicoloured forests of rooted or unrooted trees, but the number of equicolourings of a given equicolourable forest depends in a rather complicated way on the structure of the forest. In another direction, we may consider the number of trees that are equitably colourable with three (or more) colours. Again, it should be relatively easy to enumerate equitable tricolourings of trees; results for the labelled case are given by Austin [A]. But whereas a tree has just two bicolourings, and one is equitable if and only if both are, a tree with n vertices has $3 \cdot 2^{n-1}$ tricolourings, and the number of these that are equitable depends in a rather complicated way on the structure of the tree.

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